Multigrid for far and near field maps of the Helmholtz equation

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The Helmholtz equation desribes the scattering of electrons in small microscopic systems such a molecules. These problems are high-dimensional and are characterized by a smoothly varying wave number in contrast to typical engineering problems where the wave number has material jumps. Understanding these scattering process is important to basic sciences such as chemistry and biology.

In this talk we show that the far and near field scattering amplitudes for these Helmholtz equations can be efficiently be calculated using multigrid. Indeed, these amplitudes are integral expressions over the solution of the Helmholtz equation solved on a finite numerical box with absorbing boundary conditions covering the object of interest. A typical calculation has two steps. The first step is to solve the high-dimensional Helmholtz equation, which is a computationally very expensive and requires supercomputer infrastructure for the most challenging problems. The second step is to integrate over the solution to obtain the far field or near field amplitude. The latter is cheap can be done as a post processing step on a laptop.

By deforming the contour of integration into complex plane in the second step, the Helmholtz problem in the first step becomes much easier. Indeed, we show that the deformation of the contour turns the Helmholtz into a Complex shifted Laplacian problem, known to be solvable in a scalable way.

We validate the method for some benchmark problems and show the $\mathcal{O}(n)$ scalability on 3D Helmholtz and Schrödinger equations.

References

[1] Cools, S., Reps, B., and Vanroose, W. *An Efficient Multigrid Calculation of the Far Field Map for Helmholtz and Schrödinger Equations*, SIAM Journal on Scientific Computing **36** p267-395 (2014).